

Response Functions for a Granular Fluid

James DUFTY

Department of Physics, University of Florida, Gainesville, FL 32611 USA

The response of an isolated granular fluid to small perturbations of the hydrodynamic fields is considered. The corresponding linear response functions are identified in terms of a formal solution to the Liouville equation including the effects of the cooling reference state. These functions are evaluated exactly in the asymptotic long wavelength limit and shown to represent hydrodynamic modes. More generally, the linear granular Navier-Stokes equations for the response functions and related Langevin equations are obtained from an extension of Mori's identity. The resulting Green-Kubo expressions for transport coefficients are compared and contrasted with those for a molecular fluid. Next the response functions are described in terms of an effective dynamics in the single particle phase space. A closed linear kinetic equation is obtained formally in terms of a linear two particle functional. This closure is evaluated for two examples: a short time Markovian approximation, and a low density expansion on length and time scales of the mean free time and mean free path. The former is a generalization of the revised Enskog kinetic theory to include velocity correlations. The latter is an extension of the Boltzmann equation to include the effects of recollisions (rings) among the particles.

§1. Introduction

It is generally accepted that many states of driven (activated) granular matter admit a macroscopic description analogous to that of molecular fluids. Such states will be referred to as "fluidized". As with normal fluids, that continuum description can be simple or complex depending on the particular fluid considered and its state (e.g., large or small spatial gradients; near or far from boundaries; laminar or turbulent; homogeneous or heterogeneous).^{1),2)} In all cases, the basis for the macroscopic continuum description is the exact local balance equations for the relevant hydrodynamic fields, and suitable approximations for the fluxes in these equations (constitutive equations). These approximations may be based on extrapolations from experimental observations, constrained by symmetries and other known theoretical properties. The simplest case is that of a one component system for which the macroscopic fields are the density, temperature, and flow velocity. If in addition, the dimensionless spatial gradients and time derivatives are small then a Navier-Stokes hydrodynamics is expected to apply. However, the form of these equations and the dependence of their coefficients on grain properties and fluid state conditions are not known *a priori*. For granular gases, the hydrodynamic equations and explicit expressions for their coefficients can be derived from the granular Boltzmann equation. The origins of the Boltzmann equation³⁾ and a hydrodynamic description⁴⁾ can be made quite clear in this case.

At higher densities, still within the constraints of small gradients, the methods of linear response can be applied to obtain the linear Navier-Stokes equations and formally exact expressions for the transport coefficients;⁵⁾ the generalization to obtain non-linear hydrodynamics in this way has also been described.⁶⁾ The application of

linear response parallels closely its application for the same purpose to molecular fluids,^{7),8)} although significant differences appear due to the inelasticity of collisions for granular fluids. The next two sections give a brief review of the central ideas to allow the reader to see these similarities and differences. For example, an new concept of global invariants is observed with a direct connection to long wavelength hydrodynamics at the microscopic level. A new formal approach to writing equations for the response functions is given in Section 4 from an extension of the Mori projection operator method. Navier-Stokes hydrodynamics and expressions for the transport coefficients are extracted from the long wavelength form of these equations. In the second half of this presentation the practical evaluation of the response functions is considered in the context of kinetic theory. As observed elsewhere,⁹⁾ a non-trivial generalization (e.g., retaining velocity correlations) of the phenomenological Enskog kinetic theory follows directly from a short-time (Markovian) approximation. Next, the results of a systematic low density expansion are described for leading order corrections to the Boltzmann limit. The relevant length scale chosen in this expansion is the mean free path, leading to the inclusion of "ring collisions" at this order. Some outstanding problems and opportunities for the future are mentioned in the summary section.

The results described here are a personal perspective developed primarily by the author and his collaborators. The references reflect this bias, and apologies are offered to those whose excellent contributions to related topics are only recognized in the books and reviews cited here.

§2. Liouville equation and hydrodynamic modes

Attention will be restricted to the simplest realistic model of a granular fluid: a system of N smooth, inelastic, hard spheres of mass m , diameter σ , and positive normal restitution coefficient $\alpha \leq 1$. The state of the system is specified by distribution function $\rho(\Gamma)$ for the N particle phase space $\Gamma = \{\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{v}_1, \dots, \mathbf{v}_N\}$. The evolution from a given initial state is given by the Liouville equation

$$\partial_t \rho(\Gamma, t) + \bar{L} \rho(\Gamma, t) = 0. \quad (2.1)$$

The operator \bar{L} generates the hard sphere Liouville dynamics for the N particles: linear trajectories until a given pair is in contact, followed by an inelastic change in that pair's velocities, and that process continued. On each collision there is a loss of energy so the total energy for an isolated system decreases in time.¹⁰⁾ It is usual to define a temperature in terms of that energy by $E(t) \equiv 3NT(t)/2$. This is simply a definition and has no implications for an underlying thermodynamics. The decrease of $T(t)$ is represented by a cooling rate $\zeta \equiv -\partial_t \ln T$.

For an isolated system a special homogenous solution is sought in which all of the time dependence occurs through the energy, or temperature

$$\rho_h(\Gamma; n, T_h(t), \mathbf{U}) = (\ell v_0(t))^{-3N} \rho_h^* \left(\left\{ \frac{\mathbf{q}_\alpha - \mathbf{q}_\beta}{\ell}, \frac{\mathbf{v}_\alpha - \mathbf{U}_\alpha}{v_h(t)} \right\}, n \ell^3 \right), \quad (2.2)$$

where ℓ is a characteristic length scale (e.g., mean free path) and $v_0(t) = \sqrt{2T_h(t)/m}$

is the thermal velocity. This is known as the homogeneous cooling state (HCS), and is parameterized by the average density n , the temperature $T_h(t)$, and the average system velocity \mathbf{U}_α , all of which are uniform. The Γ dependence of the dimensionless distribution ρ_h^* follows from the Liouville equation

$$\bar{\mathcal{L}}\rho_h^* = 0, \quad \bar{\mathcal{L}}X \equiv \bar{L}X + \frac{1}{2}\zeta_h \sum_{\beta=1}^N \nabla_{\mathbf{v}_\beta} \cdot (\mathbf{v}_\beta X). \quad (2.3)$$

with $\mathbf{V}_\alpha = \mathbf{v}_\alpha - \mathbf{U}_\alpha$. In the definition of $\bar{\mathcal{L}}$ the cooling rate ζ_h must be determined self-consistently, i.e.

$$\int d\Gamma^* K \bar{\mathcal{L}}\rho_h^* = 0 \Rightarrow \zeta_h = \frac{2}{3n_h T_h} \int d\Gamma^* \dot{K} \rho_h^*, \quad (2.4)$$

where K is the total kinetic energy and \dot{K} is its time derivative.

For more general states a similar dimensionless distribution can be defined

$$\rho(\Gamma, t) \equiv (\ell v_0(t))^{-3N} \rho^* \left(\left\{ \frac{\mathbf{q}_\alpha}{\ell}, \frac{\mathbf{v}_\alpha - \mathbf{U}_\alpha}{v_h(t)} \right\}, n\ell^3, s \right). \quad (2.5)$$

A corresponding dimensionless time s , $\bar{\mathcal{L}}$ and ζ_h are given by

$$s = \int_0^t dt' \frac{v_h(t')}{\ell}, \quad \bar{\mathcal{L}}^* \equiv \frac{\ell}{v_h(t)} \bar{\mathcal{L}}, \quad \zeta_h^* = \frac{\ell}{v_h(t)} \zeta_h \quad (2.6)$$

If ℓ is the mean free path, then s has the interpretation of the average number of collisions in the interval $(0, t)$. The Liouville equation for ρ^* then becomes

$$(\partial_s + \bar{\mathcal{L}}^*) \rho^* = 0. \quad (2.7)$$

The definition of $\bar{\mathcal{L}}$ is such that its dimensionless form, $\bar{\mathcal{L}}^*$, is independent of s . In this representation of the Liouville equation, it is seen that the HCS is a stationary solution.

It is possible to identify a set of important eigenvalues and eigenvectors of the generator of dynamics $\bar{\mathcal{L}}^*$ by differentiating (2.3) with respect to its parameters n, T, \mathbf{U} . Actually, it is convenient to change variables from n_h and T_h to n_h and $\zeta_h(n_h, T_h)$. The result is the set of five eigenvalue equations

$$\bar{\mathcal{L}}^* \Phi_\alpha = \lambda_\alpha^* \Phi_\alpha, \quad (2.8)$$

with the eigenvalues and eigenvectors given in terms of ρ_h^*

$$\lambda_\alpha^* = \left(0, \frac{1}{2}\zeta_h^*, -\frac{1}{2}\zeta_h^*, -\frac{1}{2}\zeta_h^*, -\frac{1}{2}\zeta_h^* \right) \quad (2.9)$$

$$\Phi_1 = \frac{\partial \rho_h}{\partial n_h} |_{\zeta_h}, \quad \Phi_2 = \frac{\partial \rho_h}{\partial \zeta_h} |_{n_h}, \quad \Phi_{i=3,4,5} = \frac{\partial \rho_h}{\partial U_i}. \quad (2.10)$$

The significance of this lies in the fact that these eigenvalues are the *same* as those of the macroscopic balance equations for average number density, energy density (or temperature), and momentum density (or flow velocity) in the long wavelength limit. In this sense they represent hydrodynamic modes at the level of the Liouville equation. This is not so surprising since the corresponding modes in the elastic limit are those of the corresponding conserved quantities, all with eigenvalues 0. The elastic limit results are recovered since in that limit $\zeta_h^* \rightarrow 0$ and $\rho_h \rightarrow$ equilibrium distribution.

§3. Linear response

For molecular fluids Onsager's regression hypothesis states that the dynamics of spontaneous fluctuations in an equilibrium fluid are the same as those for the approach to equilibrium for weakly perturbed non-equilibrium states. This has been formalized by the extensive theoretical representations of linear response, and their exploration by simulations and experiment.^{7),8)} An extension of Onsager's observation to granular fluids is described here, with special attention to hydrodynamics for the large space and time scale non-equilibrium dynamics

3.1. Response functions

The objective is to describe the dynamics of the hydrodynamic fields due to small initial perturbations of the HCS. These fields are chosen to be the number density $n(\mathbf{r}, t)$, cooling rate $\zeta(\mathbf{r}, t)$, and flow velocity $\mathbf{U}(\mathbf{r}, t)$

$$y_\alpha(\mathbf{r}, t) \Leftrightarrow \{n(\mathbf{r}, t), \zeta(\mathbf{r}, t), U_3(\mathbf{r}, t), U_4(\mathbf{r}, t), U_5(\mathbf{r}, t)\}. \quad (3.1)$$

The temperature has been replaced by the local cooling rate, $\zeta(n, T) = c(n)T^{1/2}$, since the dimensionless macroscopic balance equations are diagonal in this representation in the long wavelength limit. The deviation of these fields from their values in the HCS are given by

$$\delta y_\alpha(\mathbf{r}, t) = \int d\Gamma a_\alpha(\Gamma; \mathbf{r}) (\rho(\Gamma, t) - \rho_h(\Gamma, t)), \quad (3.2)$$

where the phase functions $a_\alpha(\Gamma; \mathbf{r})$ are linear combinations of those for the local density, energy density, and momentum density; their dimensionless forms are given below. The initial state is chosen to be a "local" HCS in the sense that the state is perturbed only through the values of these hydrodynamic fields (see (2.2))

$$\rho_{\ell h}(\{y_\alpha(0)\}) \equiv \prod_{\beta=1}^N (lv(\mathbf{q}_\beta, 0))^{-3} \rho_h^* \left(\left\{ \frac{\mathbf{q}_{\alpha\gamma}}{l}, \frac{\mathbf{v}_\alpha - \mathbf{U}(\mathbf{q}_\alpha, 0)}{v_0(\mathbf{q}_\alpha, 0)} \right\}, n(\mathbf{q}_\alpha, 0) l^3 \right). \quad (3.3)$$

This can be viewed as a state for which each small cell of the fluid is in a HCS associate with the local values $\{y_\alpha(\mathbf{r}, t)\}$. It is not a solution to the Liouville equation, but rather a state whose average fields are specified as functions of \mathbf{r}, t . In this sense it is the analogue of the local equilibrium ensemble for molecular fluids.

Use of this initial state in (3.2) and expansion of $\rho_{\ell h}$ about the uniform values of $\{y_\alpha\}$ for the HCS to linear order gives the linear response

$$\delta y_\alpha(\mathbf{r}, t) = \int d\mathbf{r}' R_{\alpha\beta}(\mathbf{r}, t; \mathbf{r}', 0) \delta y_\beta(\mathbf{r}', 0). \quad (3.4)$$

The response functions are identified as

$$R_{\alpha\beta}(\mathbf{r}, \mathbf{r}', t) = \int d\Gamma a_\alpha(\Gamma, \mathbf{r}) e^{-\bar{\mathcal{L}}t} \phi_\beta(\Gamma; \mathbf{r}'). \quad (3.5)$$

with

$$\phi_\beta(\Gamma; \mathbf{r}) \equiv \sum_{i=1}^N \delta(\mathbf{q}_i - \mathbf{r}) \frac{\partial \rho_{\ell h}(\{y_\alpha(0)\})}{\partial y_\alpha(\mathbf{q}_i, 0)} \Big|_{\delta y=0}. \quad (3.6)$$

It is seen that the functions $\{\phi_\beta\}$ are just the densities associated with the hydrodynamic modes of (2.8), $\int d\mathbf{r} \phi_\beta(\Gamma; \mathbf{r}) = \Phi_\beta(\Gamma)$. This is analogous to the linear response of a molecular fluid to an initial local equilibrium state, where the perturbations are proportional to the densities associated with the conserved quantities (the long wavelength hydrodynamic modes).

It is appropriate at this point to introduce the dimensionless variables of the last section. Also, since the reference HCS is uniform the response function depends on \mathbf{r}, \mathbf{r}' only through $\mathbf{r} - \mathbf{r}'$ and a Fourier representation is convenient

$$\tilde{f}(\mathbf{k}^*) \equiv \int d\mathbf{r}^* e^{i\mathbf{k}^* \cdot \mathbf{r}^*} f(\mathbf{r}^*), \quad f(\mathbf{r}^*) = \frac{1}{V^*} \sum_{\mathbf{k}^*} e^{-i\mathbf{k}^* \cdot \mathbf{r}^*} f(\mathbf{k}^*). \quad (3.7)$$

The dimensionless response functions are then

$$\tilde{R}_{\alpha\beta}^*(\mathbf{k}^*; s) \equiv \frac{1}{V^*} \int d\Gamma^* \tilde{a}_\alpha^*(\Gamma^*, \mathbf{k}^*) e^{-\bar{\mathcal{L}}^* s} \tilde{\phi}_\beta^*(\Gamma^*; -\mathbf{k}^*) \quad (3.8)$$

with

$$\tilde{a}_\alpha^*(\Gamma^*, \mathbf{k}^*) = \sum_{s=1}^N e^{i\mathbf{k}^* \cdot \mathbf{q}_s^*} a_\alpha(\mathbf{v}_s^*), \quad a_\alpha(\mathbf{v}^*) \Leftrightarrow \left\{ 1, \frac{v^{*2}}{3} - \frac{1}{2} + \frac{\partial \ln \zeta}{\partial n^*}, \hat{\mathbf{k}}^* \cdot \mathbf{v}^*, \hat{\mathbf{e}}_1 \cdot \mathbf{v}^*, \hat{\mathbf{e}}_2 \cdot \mathbf{v}^* \right\}. \quad (3.9)$$

It follows from the definition of $\tilde{R}_{\alpha\beta}^*(\mathbf{k}^*; s)$ at $s = 0$ that $\{\tilde{a}_\alpha\}$ and $\{\tilde{b}_\alpha\}$ form a bi-orthogonal set in the sense

$$\frac{1}{V^*} \int d\Gamma^* \tilde{a}_\alpha^*(\Gamma^*, \mathbf{k}^*) \tilde{\phi}_\beta^*(\Gamma^*; -\mathbf{k}^*) = \delta_{\alpha\beta}. \quad (3.10)$$

3.2. Hydrodynamics

If the fields obey a closed set of hydrodynamic equations on large space and time scales, that dynamics must also be reflected in the dynamics of the response functions (Onsager's regression relationship)

$$\tilde{R}^*(\mathbf{k}^*; s) \rightarrow A(\mathbf{k}^*) e^{-\lambda^*(\mathbf{k}^*) s}, \quad (3.11)$$

where $\lambda^*(\mathbf{k}^*)$ is matrix whose eigenvalues are those for the hydrodynamic modes. The matrix can be given a precise representation in terms of the response functions

$$\lambda^*(\mathbf{k}^*) = -\lim (\partial_s R^*) R^{*-1}. \quad (3.12)$$

The limit indicated means long times and small k^* . A straightforward expansion to order k^{*2} leads to the Green-Kubo expressions for granular Navier-Stokes hydrodynamics. This will not be repeated here, other than to note from (3.6) that $\{\tilde{\phi}_\beta^*(\Gamma^*; -\mathbf{0}^*)\}$ are the long wavelength hydrodynamic modes of the Liouville equation so it follows directly that $\lambda_{\alpha\beta}^*(\mathbf{0}) = \lambda_\alpha^* \delta_{\alpha\beta}$,

$$\tilde{R}_{\alpha\beta}^*(\mathbf{0}; s) = e^{-\lambda_\alpha^* s} \delta_{\alpha\beta}, \quad (3.13)$$

with λ_α^* given by (2.9).

§4. Mori identity and generalized hydrodynamic equations

Formally exact equations for the response functions can be obtained by the projection operator method developed by Zwanzig and Mori.¹¹⁾ Its generalization to the granular response functions here is straightforward. To simplify the notation a matrix representation will be used and the asterisk and dependence on \mathbf{k} suppressed for the moment. Define the bi-linear functional (x, χ) by

$$(x, \chi) = \frac{1}{V} \int d\Gamma x(\Gamma) \chi(\Gamma), \quad (4.1)$$

where x and χ are from the dual spaces of a and ϕ , respectively. It is understood that dimensionless variables are used throughout so the asterisk is also suppressed. The response function is then

$$R(s) = (a(s), \phi) = (a, \phi(s)), \quad (4.2)$$

with the phase space and Liouville dynamics defined by

$$a(s) \equiv e^{\mathcal{L}s} a, \quad \phi(s) \equiv e^{-\bar{\mathcal{L}}s} \phi. \quad (4.3)$$

In this context \mathcal{L} is the adjoint of $-\bar{\mathcal{L}}$.

Define the projection operators

$$\mathcal{P}x = (x, \phi) a, \quad \mathcal{P}^\dagger \chi = \phi(a, \chi). \quad (4.4)$$

From (3.10), $(a, \phi) = 1$ and it follows that $\mathcal{P}^2 = \mathcal{P}$, $\mathcal{P}^{\dagger 2} = \mathcal{P}^\dagger$, and $(\mathcal{P}x, \chi) = (x, \mathcal{P}^\dagger \chi)$. The response function has the representations

$$R(s) = (\mathcal{P}a(s), \phi) = (a, \mathcal{P}^\dagger \phi(s)). \quad (4.5)$$

Thus the response functions depend only on the projected dynamics. Mori's identity is a decomposition of the time evolution of $a(s)$ or $\phi(s)$ into contributions from this projected dynamics and a remainder orthogonal to it (see Appendix)

$$a(s) = R(s)a + \int_0^s d\tau R(s-\tau)h(\tau), \quad h(s) = e^{\mathcal{Q}\mathcal{L}\mathcal{Q}s} \mathcal{Q}\mathcal{L}a, \quad (4.6)$$

$$\phi(s) = \phi R(s) + \int_0^s d\tau \gamma(s-\tau) R(\tau), \quad \gamma(s) = -\mathcal{Q}^\dagger e^{-\mathcal{Q}^\dagger \mathcal{L} \mathcal{Q}^\dagger s} \mathcal{Q}^\dagger \mathcal{L} \phi, \quad (4.7)$$

where $\mathcal{Q} = 1 - \mathcal{P}$. The equation for $R(s)$ now follows directly from differentiating (4.2) and use of Mori's identity

$$\partial_s R(s) + \Omega R(s) + \int_0^s d\tau \Lambda(s-\tau) R(\tau) = 0, \quad (4.8)$$

The matrices generating the dynamics are

$$\Omega = (a, \overline{\mathcal{L}}\phi), \quad \Lambda(s) = -(h(0), \gamma(s)). \quad (4.9)$$

Finally, differentiating the identities and use of (4.8) leads to new equations for $a(s)$ and $\phi(s)$

$$\partial_s a(s) + \Omega a(s) + \int_0^s d\tau \Lambda(s-\tau) a(\tau) = h(s), \quad (4.10)$$

$$\partial_s \phi(s) + \phi(s) \Omega + \int_0^s d\tau \phi(\tau) \Lambda(s-\tau) = \gamma(s). \quad (4.11)$$

The left sides of the equations represent the macroscopic or average dynamics of the response functions. The functions $h(s)$ and $\gamma(s)$ on the right sides are orthogonal to $a(s)$ and $\phi(s)$, respectively, and have the interpretation of sources for "noise". Consequently, these equations have the interpretation of generalized Langevin equations.¹¹⁾ In this context, the second equality of (4.9) represents a "fluctuation-dissipation" relation. All of the results to this point are still exact.

4.1. Hydrodynamics

The relationship of the formally exact equation (4.8) to hydrodynamics is most easily discussed in terms of the Laplace transform of the response functions

$$R(\mathbf{k}, z) \equiv \int_0^\infty ds e^{-zs} \tilde{R}(\mathbf{k}; s), \quad \text{Re } z > z_0, \quad (4.12)$$

where it is assumed that there exists some real z_0 such that $\tilde{R}_{\alpha\beta}(\mathbf{k}; s) \leq e^{-z_0 s}$ for all s . Then (4.8) gives

$$R(\mathbf{k}, z) = (z + \Omega(\mathbf{k}) + \overline{\Lambda}(\mathbf{k}, z))^{-1}, \quad (4.13)$$

where $\overline{\Lambda}(\mathbf{k}, z)$ is the Laplace transform of $\Lambda(\mathbf{k}, s)$. The zeros of $\det(z + \Omega(\mathbf{k}) + \overline{\Lambda}(\mathbf{k}, z))$ define the spectrum of $R(\mathbf{k}, z)$ and the complete dynamics of $\tilde{R}(\mathbf{k}; s)$. The spectrum for $\mathbf{k} = \mathbf{0}$ is known from the exact result (3.13) showing a set of poles at $z = -\lambda_\alpha$. Assuming only continuity in \mathbf{k} these poles shift at finite \mathbf{k} to the values $\lambda_\alpha(\mathbf{k})$ determined from

$$\det(-\lambda_\alpha(\mathbf{k}) + \Omega(\mathbf{k}) + \overline{\Lambda}(\mathbf{k}, -\lambda_\alpha(\mathbf{k}))) = 0. \quad (4.14)$$

If the dependence on \mathbf{k} is analytic then the solutions to (4.14) can be constructed as a power series, $\lambda_\alpha(\mathbf{k}) = \lambda_\alpha + k\lambda_\alpha^{(1)} + k^2\lambda_\alpha^{(2)} + \dots$. The eigenvalues truncated at order k^2 define the Navier-Stokes excitations.

The corresponding hydrodynamic equations are those of (3.11)

$$(\partial_s + \lambda(\mathbf{k})) \tilde{R}(\mathbf{k}; s) = A(\mathbf{k}), \quad (4.15)$$

with the identification of $A(\mathbf{k})$ as the residues of the hydrodynamic poles and

$$\lambda(\mathbf{k}) = \Omega(\mathbf{k}) + \bar{\Lambda}(\mathbf{k}, -\lambda(\mathbf{k})) \quad (4.16)$$

The explicit Navier-Stokes form is obtained by expanding the expressions for $\Omega(\mathbf{k})$ and $\bar{\Lambda}(\mathbf{k}, -\lambda(\mathbf{k}))$ from (4.9) to order k^2

$$\lambda(\mathbf{k}) \rightarrow \lambda + k\Omega^{(1)} + k^2 \left(\Omega^{(2)} + \bar{\Lambda}^{(2)}(z = -\lambda) \right). \quad (4.17)$$

The terms of through order k define the Euler hydrodynamics for a granular fluid, while the contributions of order k^2 define the Navier-Stokes order transport coefficients. The latter are the Green-Kubo expressions.

There are several important similarities and differences between the hydrodynamics for granular and molecular fluids. At the Euler level, there are the excitations λ which lead to a long wavelength instability not present for molecular fluids. The hydrostatic pressure has a dependence on temperature and density determined by the reference HCS distribution rather than the Gibbs distribution for a molecular fluid. Finally, there are dissipative contributions from the dependence of the cooling rate on the divergence of the flow field - a new transport coefficient.

At the Navier-Stokes level the viscous dissipation has the same form in both cases. However, Fourier's law is modified by an additional dependence of the heat flux on the gradient of the density. This can be traced to the failure of Onsager's reciprocal relations, or time reversal invariance, in the granular fluid. Finally, there are important differences in the form of the Green-Kubo expressions for transport coefficients. As an explicit example, the shear viscosity from (4.17) is found to be⁵⁾

$$\eta = -\frac{1}{V} \int d\Gamma T_{xy} \mathcal{M}_{xy} + \lim_{s \rightarrow \infty} \int_0^s ds' \int d\Gamma T_{xy} e^{-s(\bar{\mathcal{L}} + \frac{\zeta_0}{2})} \Upsilon_{xy}, \quad (4.18)$$

where the T_{ij} is the usual volume integrated momentum flux tensor, and the new flux Υ_{xy} and moment \mathcal{M}_{xy}

$$\Upsilon_{xy} = -\mathcal{Q}^\dagger \left(\bar{\mathcal{L}} + \frac{\zeta_0}{2} \right) \mathcal{M}_{xy}, \quad \mathcal{M}_{xy} = -\frac{1}{2} \sum_{r=1}^N \left(q_{r,x} \frac{\partial}{\partial v_{r,y}^*} + q_{r,y} \frac{\partial}{\partial v_{r,x}^*} \right) \rho_h. \quad (4.19)$$

There are two parts, a time integral of a flux-flux correlation function as in the usual expressions for molecular fluid, and a time-independent contribution. Both terms occur in the elastic limit, with the latter being a peculiarity of the hard sphere interaction. However, for the granular fluid this expression occurs even for continuous particle interactions and is due to the absence of time reversal invariance. Also in the elastic limit the flux $\Upsilon_{xy} \rightarrow T_{xy}$ and the correct Green-Kubo expression for the viscosity of a hard sphere fluid is regained. However, the granular fluid flux $\Upsilon_{xy} \neq T_{ij}$. Instead one of the fluxes is associated with the local conserved densities

\tilde{a}_α of (3.9) while the other flux is associated with the bi-orthogonal densities $\tilde{\phi}_\beta$ of (3.6). Finally, it is noted that the flux-flux correlation function has the invariant subspace of the dynamics projected out, a necessary condition for the convergence of the time integral for large s .

§5. Kinetic theory of response functions

Practical evaluation of the response functions for all \mathbf{k}, s is a formidable task for both molecular and granular fluids. In the former case, phenomenological approaches based on modeling "memory functions" in terms of a few moments has met with considerable success.¹²⁾ More controlled and detailed descriptions are provided by kinetic theory. In this section the representation of response functions appropriate for such methods is given.⁹⁾ Subsequently, two practical approximations are described.

The Fourier transformed response function can be written in the alternative form

$$\tilde{R}_{\alpha\beta}(\mathbf{k}; s) = \int d\Gamma \tilde{a}_\alpha(\Gamma, \mathbf{k}) e^{-\bar{\mathcal{L}}s} \phi_\beta(\Gamma; \mathbf{r} = \mathbf{0}). \quad (5.1)$$

Then, since the local densities $\tilde{a}_\alpha(\Gamma, \mathbf{k})$ are sums of single particle functions (see (3.9)), integration over all degrees of freedom except those for one particle can be performed to get a representation in the single particle phase space

$$\tilde{R}_{\alpha\beta}(\mathbf{k}; s) = n \int d\mathbf{v}_1 d\mathbf{q}_1 e^{i\mathbf{k} \cdot \mathbf{q}_1} a_\alpha(\mathbf{v}_1) \phi_\alpha^{(1)}(x_1; \mathbf{r} = \mathbf{0}, s), \quad (5.2)$$

The reduced density $\phi_\alpha^{(1)}(x_1; \mathbf{0}, s)$ is a member of a set defined by

$$n^m \phi_\alpha^{(m)}(x_1, \dots, x_m; \mathbf{0}, s) = \frac{N!}{(N-m)!} \int dx_{m+1} \dots dx_N e^{-\bar{\mathcal{L}}s} \phi_\alpha(\Gamma; \mathbf{0}). \quad (5.3)$$

Here $x_i = \mathbf{q}_i, \mathbf{v}_i$ denotes a point in the six dimensional phase space for a single particle. These functions obey a hierarchy of equations obtained by direct differentiation. The first of these equations describes the dynamics of the single particle function $\phi_\alpha^{(1)}(x_1; \mathbf{0}, s)$

$$\left(\partial_s + \frac{1}{2} \zeta(3 + \mathbf{v}_1 \cdot \nabla_{\mathbf{v}_1}) + \mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} \right) \phi_\alpha^{(1)} = n\sigma^2 \int dx_2 \bar{T}(1, 2) \phi_\alpha^{(2)}(x_1, x_2, s), \quad (5.4)$$

where $\bar{T}(1, 2)$ is the binary collision operator describing velocity changes due to hard sphere interactions (its detailed form^{13), 14)} is not needed here). Equation (5.4) shows the coupling of $\phi_\alpha^{(1)}$ to the two particle function $\phi_\alpha^{(2)}$, which in turn obeys an equation coupled to $\phi_\alpha^{(2)}$; hence the structure of a hierarchy. A closed *kinetic equation* for $\phi_\alpha^{(1)}$ results from this first hierarchy equation if $\phi_\alpha^{(2)}$ can be expressed approximately as a functional of $\phi_\alpha^{(1)}$

$$\phi_\alpha^{(2)}(x_1, x_2, s) \simeq \Phi(x_1, x_2, s | \phi_\alpha^{(1)}). \quad (5.5)$$

Use of this functional in (5.3) gives the desired kinetic equation, and its solution gives the response function via (5.2).

Generally, such a functional relationship entails limitations of space and time scales, density or other conditions for validity. An example is the Markovian approximation. This represents the functional by its exact form at $s = 0$

$$\Phi(x_1, x_2, s \mid \cdot) \rightarrow \Phi(x_1, x_2, s = 0^+ \mid \cdot). \quad (5.6)$$

This is a type of mean field approximation, representing the collisional process by its average value in the initial state of the system. It is therefore exact at short times but only approximate thereafter. For the hard sphere interactions considered here, it describes the non-trivial binary collisions, modified by correlations with the environment. It neglects dynamical correlations that develop over longer times. The detailed form of the Markovian approximation is worked out elsewhere⁹⁾ and only the result is quoted here. Equation (5.4) becomes the kinetic equation

$$\left(\partial_s + \frac{1}{2} \zeta \nabla_{\mathbf{v}_1} \cdot \mathbf{v}_1 + \mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} + \hat{I} \right) \phi_\alpha^{(1)} = 0, \quad (5.7)$$

where the collision operator is given by

$$\begin{aligned} \hat{I} \phi_\alpha^{(1)} &= \int dx_{s+1} \bar{T}(1, 2) \Phi(x_1, x_2, s = 0^+ \mid \phi_\alpha^{(1)}) \\ &= - \int dx_2 \bar{T}(x_1, x_2) g_h^{(2)}(x_1, x_2) \left[f_h^{(1)}(v_1) \phi_\alpha^{(1)}(x_2, s) + f_h^{(1)}(v_2) \phi_\alpha^{(1)}(x_1, s) \right] \\ &\quad - \int d\mathbf{q}_2 c_\lambda(\mathbf{v}_1, \mathbf{q}_{12}) \frac{1}{n_h} \int d\mathbf{v}_2 a_\lambda(\mathbf{v}_2) \phi_\alpha^{(1)}(x_2, s). \end{aligned} \quad (5.8)$$

The function $g_h^{(2)}(x_1, x_2)$ describes the pair correlations in the HCS (including velocity correlations), and $c_\lambda(\mathbf{v}_1, \mathbf{q}_{12})$ is related to its functional derivative with respect to the local hydrodynamic fields $y_\lambda(\mathbf{q}_2)$

$$c_\lambda(\mathbf{v}_1, \mathbf{q}_{12}) = \int dx \bar{T}(x_1, x) f_h^{(1)}(v_1) f_h^{(1)}(v) \left[\frac{\delta g_h^{(2)}[x_1, x | \delta y]}{\delta y_\lambda(\mathbf{q}_2)} \right]_{\delta y=0}. \quad (5.9)$$

The corresponding response functions are determined from the Fourier transform of this equation, with the result

$$\tilde{R}_{\alpha\beta}(\mathbf{k}; s) = n \int d\mathbf{v}_1 a_\alpha(\mathbf{v}_1) e^{(i\mathbf{k} \cdot \mathbf{v} - \tilde{I}(\mathbf{k}) - \frac{1}{2} \zeta \nabla_{\mathbf{v}_1} \cdot \mathbf{v}_1)s} \frac{\delta f_{\ell h}^{(1)}}{\delta y_\beta} \Big|_{\delta y=0}, \quad (5.10)$$

where $\tilde{I}(\mathbf{k})$ is the Fourier representation for the collision operator \hat{I} , and the initial condition is the functional derivative of the single particle distribution $f_{\ell h}^{(1)}$ determined from the local HCS distribution (3.3).

The Markovian approximation leads to a practical result, without *a priori* limitations on the density, or length scale. Thus it can be applied to both dilute and dense fluid conditions, from hydrodynamic length scales to those smaller than the grain size. In the elastic limit it reduces to the generalized Enskog approximation that has met with great success in that diverse context.^{7), 12)} For Granular fluids,

the required input property $g_h^{(2)}(x_1, x_2)$ is not known and hence most applications to date have used the further approximation of neglecting the velocity correlations. Still, the results provide an accurate and practical extension of the Boltzmann results to finite density gases.

§6. Response at Low Density

A second example of a kinetic theory description for response can be obtained more systematically using a dimensionless density as expansion parameter. The starting point is the hierarchy for the reduced distribution functions $f^{(m)}(x_1, \dots, x_m, s)$ associated N particle distribution function evolving from the initial local HCS distribution (3.3)

$$n^m f^{(m)}(x_1, \dots, x_m; s) = \frac{N!}{(N-m)!} \int dx_{m+1} \dots dx_N e^{-\bar{\mathcal{L}}s} \rho_{\ell h}(\{y_\alpha(0)\}). \quad (6.1)$$

It follows that the function $\phi_\alpha^{(1)}(x_1; \mathbf{r} = \mathbf{0}, s)$ that determines the response functions in (5.2) is obtained from $f^{(1)}(x_1, s)$ by functional differentiation

$$\phi_\alpha^{(1)}(x_1; \mathbf{r} = \mathbf{0}, s) = \left[\frac{\delta f^{(1)}(x_1; s)}{\delta y_\alpha(\mathbf{0})} \right]_{\delta y=0}. \quad (6.2)$$

The analysis proceeds by first finding a kinetic equation for $f^{(1)}$ and then determining the corresponding kinetic equation for $\phi_\alpha^{(1)}$ by functional differentiation. Only an outline of the results is provided here, with further details¹⁵⁾ to be given elsewhere.

The first hierarchy equation is¹⁶⁾

$$\left(\partial_s + \frac{1}{2} \zeta \nabla_{\mathbf{v}_1} \cdot \mathbf{v}_1 + \mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} \right) f^{(1)}(x_1; s) = \int dx_2 \bar{T}(1, 2) f^{(2)}(x_1, x_2; s). \quad (6.3)$$

A kinetic equation is obtained by finding a functional relationship $f^{(2)}(x_i, x_j; s) = F^{(2)}(x_i, x_j, s | f^{(1)})$. This is accomplished as an expansion in the parameter σ/ℓ , where σ is the grain diameter and $\ell = 1/n\sigma^2$ is the mean free path, for $\sigma/\ell \ll 1$. The hierarchy equations can then be solved formally for $f^{(m)}$ as a power series in this small parameter. The solutions can be inverted to give a representation of $f^{(m)}$ in terms of $f^{(1)}$ and the initial conditions. The result is

$$F^{(2)}(x_1, x_2; s | f^{(1)}) = f^{(1)}(x_1; s) f^{(1)}(x_2; s) + \left(\frac{\sigma}{\ell} \right)^2 C^{(2)}(x_1, x_2; s | f^{(1)}) + \dots \quad (6.4)$$

where $C^{(2)}$ is determined from

$$\left(\partial_s + \mathcal{L} \left(1 | f^{(1)} \right) + \mathcal{L} \left(2 | f^{(1)} \right) \right) C^{(2)}(x_1, x_2; s | f^{(1)}) = \bar{T}(1, 2) f^{(1)}(x_1; s) f^{(1)}(x_2; s). \quad (6.5)$$

The single particle generator $\mathcal{L}(1 | f^{(1)})$ is

$$\begin{aligned} \mathcal{L}(1 | f^{(1)}) X(1) = & \left(\mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} + \frac{1}{2} \zeta \nabla_{\mathbf{v}_1} \cdot \mathbf{v}_1 \right) X(1) \\ & - \int dx_3 \bar{T}(1, 3) \left(f^{(1)}(x_1; s) X(x_3) + X(x_1) f^{(1)}(x_3; s) \right). \end{aligned} \quad (6.6)$$

These results determine the functional $F^{(2)}(x_1, x_2; s | \cdot)$ exactly to order $(\sigma/\ell)^2$. For the special case $\delta y_\alpha = 0$ in (6.1), these equations become time independent and determine the one and two particle reduced distribution functions for the HCS at low density. Closely related equations have been studied to determine pair correlations in the HCS¹⁸⁾

To expose the content of this result, the linear equation for $C^{(2)}$ can be solved

$$\begin{aligned} C^{(2)}(x_1, x_2; s | f^{(1)}) = & \mathcal{U}(s, 0) \left[f_{\ell h}^{(2)}(x_1, x_2) - f_{\ell h}^{(1)}(x_1) f_{\ell h}^{(1)}(x_2) \right] \\ & + \int_0^s ds' \mathcal{U}(s, s') \bar{T}(1, 2) f^{(1)}(x_1; s') f^{(1)}(x_2; s'), \end{aligned} \quad (6.7)$$

where the solution operator $\mathcal{U}(s, s')$ obeys the equation

$$\left(\partial_s + \mathcal{L}(x_1 | f^{(1)}) + \mathcal{L}(x_2 | f^{(1)}) \right) \mathcal{U}(s, s') = 0, \quad \mathcal{U}(s', s') = 1. \quad (6.8)$$

With these results, the first hierarchy equation (6.3) becomes

$$\begin{aligned} \left(\partial_s + \frac{1}{2} \zeta \nabla_{\mathbf{v}_1} \cdot \mathbf{v}_1 + \mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} \right) f^{(1)}(x_1; s) = & \int dx_2 \bar{T}(1, 2) f^{(1)}(x_1; s) f^{(1)}(x_2; s) \\ & + \left(\frac{\sigma}{\ell} \right)^2 \int_0^s ds' \int dx_2 \bar{T}(1, 2) \mathcal{U}(s, s') \bar{T}(1, 2) f^{(1)}(x_1; s') f^{(1)}(x_2; s') \\ & + \left(\frac{\sigma}{\ell} \right)^2 \int dx_2 \bar{T}(1, 2) \mathcal{U}(s, 0) \left[f_{\ell h}^{(2)}(x_1, x_2) - f_{\ell h}^{(1)}(x_1) f_{\ell h}^{(1)}(x_2) \right] \end{aligned} \quad (6.9)$$

To lowest order, the first term on the right side gives the granular nonlinear Boltzmann kinetic equation. This approximation has been studied in some detail for low density granular gases.^{2), 17)} The second term on the right side describes "ring collisions", which are dynamically correlated recollisions among pairs due to sequential collisions with many other particles. Finally, the last term describes related dynamical correlations due to initial static correlations in the initial local HCS.

The *linear* kinetic equation for $\phi_\alpha^{(1)}$ to determine the response functions follows from (6.2), functional differentiation of (6.9), and setting $\delta y_\alpha = 0$. It has the structural form

$$(\partial_s + \mathcal{L}_h(x_1)) \phi_\alpha^{(1)}(x_1; s) + \int_0^s ds' \mathcal{R}(s - s') \phi_\alpha^{(1)}(x_1; s') = I_\alpha(x_1; s), \quad (6.10)$$

where the source I_α is due to the evolution of initial pair correlations, inherited from the last term of (6.2). The operator $\mathcal{L}_h(1)$ is the generator for dynamics of the linear granular Boltzmann equation

$$\begin{aligned} \mathcal{L}_h(x_1) X(x_1) = & \left(\mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} + \frac{1}{2} \zeta_h (3 + \mathbf{v}_1 \cdot \nabla_{\mathbf{v}_1}) \right) X(x_1) \\ & - \int dx_3 \bar{T}(1, 3) \left(f_h^{(1)}(v_1) X(x_3) + X(x_1) f_h^{(1)}(v_3) \right). \end{aligned} \quad (6.11)$$

It can be shown that $\mathcal{L}_h(1)$ is the low density limit of the generator for the Markovian approximation (5.7). The last term on the left side of (6.10) represents the correlated collisions generated by the linear ring operator $\mathcal{R}(s)$, and the source on the right side is due to the dynamical evolution of initial pair correlations. Both of these terms are proportional to $(\sigma/\ell)^2$. Their detailed forms are lengthy and will not be given here. In the elastic limit, they reduce to the ring kinetic theory for response functions of a molecular fluid.

The most interesting feature of the ring operator is its description of a mechanism for slow dynamics not present at the level of the Boltzmann equation. It is due to a coupling of hydrodynamic modes that originates from the generator $e^{-(\mathcal{L}_h(x_1) + \mathcal{L}_h(x_2))s}$ in the solution to (6.8). It is well known that the hydrodynamic modes of a molecular fluid are contained in the spectrum of the linearized Boltzmann operator, and a similar result has been proved for the linearized granular Boltzmann equation.¹⁹⁾ Thus in general the action of this operator generates the exponential decay of two hydrodynamic modes at all possible wavelengths, leading to slow decay (algebraic, logarithmic) of response functions for molecular fluids. Similar slow decay has been predicted on more phenomenological "mode coupling" methods for the related flux correlation functions in granular fluids.²²⁾ The above kinetic equation provides the means to investigate this mechanism in more detail and broader context.

A Laplace transform of (6.10) and its formal solution leads to the Fourier and Laplace transformed response functions in the form

$$R(\mathbf{k}, z) = n \int d\mathbf{v} a(\mathbf{v}) \left(z + \mathcal{L}_h(\mathbf{k}) + \bar{\mathcal{R}}(\mathbf{k}, z) \right)^{-1} \left(\Phi^{(1)}(\mathbf{v}) + \bar{I}_0(\mathbf{v}, \mathbf{k}, z) \right). \quad (6.12)$$

where $\Phi^{(1)}(\mathbf{v})$ is the reduced single particle function determined from the global invariant Φ in (2.10). An important consequence of the eigenvalue equation (2.8) for the Liouville equation is that these same long wavelength eigenvalues are poles of the resolvent operator in (6.12)

$$(\mathcal{L}_h(\mathbf{0}) + \bar{\mathcal{R}}(\mathbf{0}, -\lambda_\alpha)) \Phi_\alpha^{(1)} = \lambda_\alpha \Phi_\alpha^{(1)}. \quad (6.13)$$

Assuming analyticity in the wavevector \mathbf{k} this assures the existence of hydrodynamic excitations in the spectrum of $\mathcal{L}_h(\mathbf{k}) + \bar{\mathcal{R}}(\mathbf{k}, z)$. Then by perturbation theory¹⁹⁾ the hydrodynamic modes, including effects of the ring collisions, can be explored through Navier-Stokes order.

§7. Summary

The presentation here has given an overview of linear response functions for excitations in the HCS or a granular fluid. The HCS is the homogeneous state of

an isolated fluid, corresponding to the equilibrium state or a molecular fluid, and is perhaps the simplest case to consider. The response for states of more practical interest (steady shear or other driven steady states) is considerably more complex, and relatively little is known even in the case of molecular fluids. Here, an attempt was made to show the structural features that are the same for granular and molecular fluids, while attending to their differences in detail.

Although the utility of these functions to describe hydrodynamic response has been emphasized, there application for shorter length and time scale phenomena should be recognized. There are many methods for practical evaluation suggested by experience with molecular fluids. The kinetic theory approach has been illustrated here with the Markovian approximation that encompasses all length and time scales and a range of densities well beyond the Boltzmann limit. In addition, systematic corrections to the Boltzmann limit have been described for low density granular gases to include the novel effects of correlated many-body collisions (rings). Still to be explored are the consequences of this low density kinetic theory, particularly the consequences of hydrodynamic mode coupling in the spectrum of the ring operator. While this is well known for molecular fluids, there is a qualitative difference in the hydrodynamic modes for granular gases. Some of the modes are unstable (in dimensionless form) and there is the potential for a qualitative difference in the hydrodynamic dispersion relations determined from $R(\mathbf{k}, z)$. This occurs for molecular fluids in two dimensions, due to mode coupling effects, and may be more significant for granular fluids in all dimensions due to the unstable modes. The detailed evaluation of (6.12) will clarify this possibility.

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Appendix A

— Mori's identity —

The projection operators of (4.4) are $\mathcal{P}x = (x, \psi) a$, $\mathcal{P}^\dagger \chi = \phi(a, \chi)$. Let $\mathcal{Q} = 1 - \mathcal{P}$ and $\mathcal{Q}^\dagger = 1 - \mathcal{P}^\dagger$ denote the corresponding orthogonal projections. Then $a(s)$ can be decomposed as

$$a(s) = (\mathcal{P} + \mathcal{Q}) a(s) = R(s)a + a_\perp(s), \quad (\text{A.1})$$

where $a_\perp(s) = \mathcal{Q}a(s)\mathcal{Q}$. Next operator with \mathcal{Q} on the equation of motion $(\partial_s - \mathcal{L}) a(s) = 0$, to get

$$(\partial_s - \mathcal{Q}\mathcal{L}\mathcal{Q}) a_\perp(t) = \mathcal{Q}\mathcal{L}\mathcal{P}a(t) = R(s)\mathcal{Q}\mathcal{L}a. \quad (\text{A.2})$$

The solution is

$$a_\perp(t) = \int_0^s d\tau R(s - \tau) e^{\hat{\mathcal{L}}\tau} \mathcal{Q}\mathcal{L}a, \quad (\text{A.3})$$

and its substitution into (A.1) gives Mori's identity (4.6). A similar analysis for $\psi(s)$ gives the identity (4.7).

Finally, differentiating the response function and using Mori's identity gives

$$\begin{aligned}\partial_s R(s) &= R(s) (\mathcal{L}a, \phi) + \int_0^s d\tau R(s-\tau) (\mathcal{L}h(\tau), \phi) \\ &= - (a, \overline{\mathcal{L}}\phi) R(s) - \int_0^s d\tau (a, \overline{\mathcal{L}}\gamma(s-\tau)) R(\tau)\end{aligned}\quad (\text{A.4})$$

The first equality comes from using the form $(a(s), \phi)$ while the second results from the form $(a, \phi(s))$.

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